

**Focus Report**  
**New Chemicals Program**  
PMN Number: **T-11-0012**

Focus Date: 08/28/2011 11:00:00 PM Report Status: Completed  
Consolidated Set:  
Focus Chair: Jim Alwood Contractor: Stephen Wieroniey

**I. Notice Information**

Submitter: Shell Chemical LP CAS Number: 1197343-01-3  
Chemical Name: Distillates (Fischer-Tropsch), C10-20-branched and linear Definition: A complex combination of hydrocarbons obtained from a feedstock derived from the catalytic hydrogenation of carbon monoxide (the Fischer-Tropsch Process), optionally followed by one or more of the following processes: hydrotreatment, hydroisomerization, hydrocracking. It consists predominantly of branched and linear aliphatic hydrocarbons having carbon numbers in the range of C 10 to C20 and boiling in the range of approximately 200°C to 310°C (392°F to 590°F).  
Use: Gas to Liquids (GTL) base oil used for drilling fluids. Guar polymer and/or proppant carrier for hydraulic fracturing. No references were found for this material. [REDACTED]  
Other Uses: [REDACTED]  
PV-Max: 25,000,000 Kg/yr  
Manufacture: Import: X

**II. SAT Results**

(1) **Health Rating:** 1-2 **Eco Rating:** 3 **Comments:** ;  
**Occupational:** 2-3C **Non-Occupational:** **Environmental:** 3  
(1) **PBT:** 2 2 1 **Comments:** PMN

**III. OTHER FACTORS**

**Categories:**

Health Chemical Category: Ecotox SAR and TSCA New Chemical Category: neutral organic chemicals; Neutral Organics

**Related Cases/Regulatory History:**

Health related Cases: [REDACTED]  
Ecotox Related Cases: Analogs: [REDACTED]  
Regulatory History: [REDACTED]  
[REDACTED]-FOCUS DROP  
[REDACTED]-PENDING A NON-5(e) SNUR  
[REDACTED]-FOCUS DROP/LETTER  
[REDACTED]-FOCUS DROP/LETTER  
[REDACTED]-PENDING TESTING

**MSDS/Label Information:**

MSDS: No Label: No

**Exposure Based Information:**

Exposure Based Review: N Exposure Based Review (Health): N  
Exposure Based Review (Eco): Y Exposure Based (Occupational): No  
Exposure Based Review (Non Occupational): N Exposure Based (Environmental): Y

Exposure Parameter	Exposure-Based	Persistent/Bioaccum	Exposure Value
Surface DW:		Yes	
Fish Ingestion:			
Ground DW:	Yes	Yes	21.7
Inhalation:	Yes	Yes	0.0928
Water Releases:	Yes	Yes	0.00857
Total Releases:	Yes	Yes	2510225
Consumer Exposure:	Yes	Yes	25057420.3165

#### IV. Summary of SAT Assessment

##### Fate:

###### Fate Summary:

T-11-0012

FATE: Estimations for low weight 5-ethyl-2-methyl-heptane, C<sub>10</sub>H<sub>22</sub>, MW 142.29

Liquid with MP = -33C (M, PMN)

log Kow = 5.11 (E);

S = 1.14 mg/L at 25 C (E)

VP = 0.449 torr at 25 C (E)

BP = 203-335 C (M, PMN)

H = 5.3 (E)

log Koc = 3.05 (E)

log Fish BCF = 3.04 (E)

log Fish BAF = 2.954 (E)

POTW removal (%) = 90-99 via sorption, stripping, and biodeg; Analog(Saralene 185V):

OECD306(SW

Biodeg - Closed Btl): 62%/28d; Analog(SMDS-2): OECD 301F(Mano Resp): 75%/28d, 60%/10d; OECD 305(BCF): LogBCF=3.2(dry weight), 4.5(lipid weight).

Time for complete ultimate aerobic biodeg = wk to > mo

Sorption to soils/sediments = moderate-strong

Volatilization half-life from a standard river = 1 hr

Volatilization half-life from a standard lake = 5 da

Atmospheric Oxidation Half-life = 11 hrs via OH radical

PBT Potential: P2B2

\*CEB FATE: Migration to ground water = slow-moderate

##### Health:

###### Health Summary:

Absorption is poor all routes based on physical/chemical properties and analogs. There is concern for eye and skin irritation, more severe with repeated exposure ( ); dermal sensitization ( ) and a submitted study); reproductive toxicity ( ); possible liver toxicity ( ) and lung toxicity in the form of chemical pneumonia. Low moderate concern.

###### Test Data:

(-) Salmonella with and without activation; (-) E. coli with and without activation; no eye irritation in rabbits; no skin irritation in rabbits; rat oral LD<sub>0</sub> = 5000 mg/kg; rabbit dermal LD<sub>0</sub> = 5000 mg/kg; rat inhalation LC<sub>0</sub> = 2.19 mg/L; (+) for skin sensitization in a mouse local lymph node assay at 100 % ai but not at 50% ai

28-day dermal study in rabbits dosed with 2 mL/kg, progressive skin irritation

dermal sensitizer in humans

rat oral devel/repro screen LOEL = 100 mg/kg, mild liver changes at all doses

rat oral devel/repro screen NOEL = 150 mg/kg, lower fertility index with a longer mean mating time at 1000 mg/kg

: mild eye irritation in rabbits; mild skin irritation in rabbits

##### Ecotox:

###### Ecotox Values:

Fish 96-h LC<sub>50</sub>: 0.19(P)

Daphnid 48-h LC<sub>50</sub>: 0.14(P)

Green algal 96-h EC<sub>50</sub>: 0.17(P)

Fish Chronic Value: 0.026(P)  
Daphnid ChV: 0.031(P)  
Algal ChV: 0.17(P)

**Ecotox values comments:** Predictions are based on SARs for neutral organic chemicals; SAR chemical class = hydrocarbon; MW 142 (low weight); log Kow = 5.11 (EPI, low weight); liquid with mp = -33 C (M); S = 1.1 mg/L (P, low weight); pH7; effective concentrations based on 100% active ingredients and nominal concentrations; DW hardness < 150.0 mg/L as CaCO<sub>3</sub>; and DW TOC <2.0 mg/L;

**Ecotox Factors:**

Assessment Factor: 10  
Concern Concentration:  
- Acute Value  
Concern Concentration: 3  
- Chronic Value

## V. Summary of Exposures/Releases

Engineering Summary: T-11-0012

Exposures/Releases	Release	Release	Release
Scenario	Use: Drilling Fluid or Proppant Carrier for Hydraulic Fracking	Use: Drilling Fluid or Proppant Carrier for Hydraulic Fracking	Use: Drilling Fluid or Proppant Carrier for Hydraulic Fracking
Sites	125	125	125
Media	Air	Water or Incineration or Landfill	Air
Descriptor A	Typical	High End	Output 2
Quantity A (Release = kg/site/day; Exposure = mg/day)	8.4E-3	3.8E+1	3.3E-6
Frequency A (day/year)	40	11	40
Descriptor B	Worst Case		
Quantity B (Release = kg/site/day; Exposure = mg/day)	1.7E-2		
Frequency B (day/year)	40		
From	Unloading Liquid Raw Material from Tank Trucks	Cleaning Liquid Residuals from Tank Trucks Used to Transport the Raw Material	Cleaning Liquid Residuals from Tank Trucks Used to Transport the Raw Material
Workers			
Exposure Type			

Engineering Summary: Exposures/Releases	Release	Release	Release
Scenario	Use: Drilling Fluid or Proppant Carrier for Hydraulic Fracking	Processing: Bulk Liquid Transfer	Processing: Bulk Liquid Transfer
Sites	125	1	1
Media	Water or Incineration or Landfill	Air	Water
Descriptor A	Output 2	Typical	High End
Quantity A (Release = kg/site/day; Exposure = mg/day)	5.0E+3	3.4E-1	2.0E+2
Frequency A (day/year)	40	250	250
Descriptor B		Worst Case	
Quantity B (Release = kg/site/day; Exposure = mg/day)		3.4E-1	
Frequency B (day/year)		250	
From	Disposal of Drilling Fluid	Unloading Liquid Raw Material from Ship	Cleaning Liquid Residuals from Tank Trucks Used to Transport the Raw Material
Workers			
Exposure Type			

## V. Summary of Exposures/Releases

Engineering Summary: T-11-0012

Exposures/Releases	Release	Exposure	Exposure
<b>Scenario</b>	<b>Processing: Bulk Liquid Transfer</b>	<b>Use: Drilling Fluid or Proppant Carrier for Hydraulic Fracking</b>	<b>Use: Drilling Fluid or Proppant Carrier for Hydraulic Fracking</b>
<b>Sites</b>	<b>1</b>	<b>125</b>	<b>125</b>
<b>Media</b>	<b>Air</b>	<b>Dermal</b>	<b>Inhalation</b>
Descriptor A	Output 2	High End	Worst Case
Quantity A (Release = kg/site/day; Exposure = mg/day)	1.2E-3	1.8E+3	5.6E+1
Frequency A (day/year)	250	200	200
Descriptor B			Typical
Quantity B (Release = kg/site/day; Exposure = mg/day)			4.0E+0
Frequency B (day/year)			200
From	Cleaning Liquid Residuals from Tank Trucks Used to Transport the Raw Material	Unloading Liquid Raw Material from Tank Trucks	Unloading Liquid Raw Material from Tank Trucks
Workers		600	600
Exposure Type		Liquid	Vapor

<b>Engineering Summary: Exposures/Releases</b>	<b>Exposure</b>	<b>Exposure</b>	
<b>Scenario</b>	<b>Processing: Bulk Liquid Transfer</b>	<b>Processing: Bulk Liquid Transfer</b>	
<b>Sites</b>	<b>1</b>	<b>1</b>	
<b>Media</b>	<b>Dermal</b>	<b>Inhalation</b>	
Descriptor A	High End	Worst Case	
Quantity A (Release = kg/site/day; Exposure = mg/day)	1.8E+3	4.9E+3	
Frequency A (day/year)	250	250	
Descriptor B		Typical	
Quantity B (Release = kg/site/day; Exposure = mg/day)		1.6E+2	
Frequency B (day/year)		250	
From	Unloading Liquid Raw Material from Ship	Unloading Liquid Raw Material from Ship	
Workers	3	3	
Exposure Type	Liquid	Vapor	

## **VI. Focus Decision and Rationale**

### **Regulatory Actions**

Regulatory Decision: TME Denial

Decision Date: 08/28/2011

Type of Decision:

Rationale:

T-11-0012 was denied for human health and ecotoxicity concerns. The submitter must offer a reason why this submission should qualify as a test market. Human health concerns were low-moderate. Potential concerns were from dermal exposure, risks were mitigated by dermal PPE listed in the MSDS. There are concerns for health effects from potential inhalation exposure. Ecotoxicity concerns were high. Risks to the environment were high due to exceedences of the acute and chronic COC during the release period. The SWCs of 2577.32 ppb and 4.75E+05 ppb exceeded the 28 ppb during processing and use operations respectively. The 3 ppb chronic COC was exceeded 68/250 release days and 40/40 release days during processing and use operations respectively. The following CEB exposure based criteria was met: Drinking (Surface) Water Dose (3.85E-02mg/kg/day), Fish Ingestion Dose (1.80E-01 mg/kg/day), Groundwater Dose (9.28E-02 mg/kg/day), Surface Water Release After Treatment (2.51E+06 kg/yr) and Total Release After Treatment (2.51E+07kg/yr).

COC: Chronic – 3 ppb; Acute – 28 ppb

Summary of Exposures and Releases:

Proc:

1 site, 250 days/year, 3 workers

Inhalation: Vapor: Typical: 1.6E+2 mg/day; Worst Case: 4.9E+3 mg/day

Dermal: 1.8E+3 mg/day (Liquid 100%)

Releases to Water: 2.0E+2 kg/site-day over 250 days/yr

Releases to Air 1: Typical: 3.4E-1 kg/site-day over 250 days/yr; Worst Case: 3.4E-1 kg/site-day

Releases to Air 2: 1.2E-3 kg/site-day over 250 days/yr

Fate Releases to Water (90% Removal)

SWC: 2577.32 ppb

DW: LADD: 2.70E-03 mg/kg/day; ADR: 0.13 mg/kg/day

FI: LADD: 1.26E-02 mg/kg/day; ADR: 0.99 mg/kg/day

>COC (3 ppb) 68/250 release days

Fate Release to Air:

Fugitive Air: LADD: 1.88E-04 mg/kg/day; ADR: 8.57E-03 mg/kg/day

Use:

125 sites, 40 days/year, 600

Inhalation: Vapor: Typical: 4.0E+0 mg/day; Worst Case: 5.6E+1 mg/day

Dermal: 1.8E+3 mg/day (Liquid 100%)

Releases to Water 1: 3.8E+1 kg/site-day over 11 days/yr

Or Incineration or Landfill

Releases to Water 2: 5.0E+3 kg/site-day over 40 days/yr

Or Incineration or Landfill

Releases to Air 1: Typical:

Typical: 8.4E-3 kg/site-day over 40 days/yr; Worst Case: 1.7E-2 kg/site-day over 40 days/yr

Releases to Air 2: 3.3E-6 kg/site-day over 40 days/yr

Fate Releases to Water (90% Removal)

SWC: 4.75E+05 ppb

DW: LADD: 1.07E-02 mg/kg/day; ADR: 21.70 mg/kg/day

FI: LADD: 4.98E-02 mg/kg/day; ADR: 88.80 mg/kg/day

>COC (3 ppb) 40/40 release days

Fate Release to Air:

Fugitive Air: LADD: 1.50E-06 mg/kg/day; ADR: 4.27E-04 mg/kg/day

Stack Air: LADD: 5.43E-05 mg/kg/day; ADR: 6.23E-03 mg/kg/day

Fate Releases to Landfill: LADD: 9.28E-02 mg/kg/day

P2 Rec Comments:

**Testing:**

**Prefocus Recommended:**

Health:

similar to HPV chemicals/categories

**Final Recommended:**

Health:

Eco:

Fate:

Other:

**SAT Report**  
PMN Number: **T-11-0012**  
SAT Date: **8/12/2011**  
Print Date: **12/4/2015**

**Related cases:**

Health related cases:

Ecotox related cases:    Analogs:

**Concern levels:**

Type of Concern:	<u>Health</u>	<u>Eco</u>	<u>Comments</u>
Level of Concern:	1-2	3	

<u>Persistence</u>
2

<u>Bioaccum</u>
2

<u>Toxicity</u>
1

Comments

PMN

**Exposure Based Review:**

**Health:** No    **Exposure based testing (health):** similar to HPV chemicals/categories

**Ecotox:** Yes

**Routes of exposure:**

**Health:** Dermal Inhalation

**Ecotox:** All releases to water

**Fate:** ;

**Keywords:**

**Keywords:** LIVER; LUNG; IRR-S; E; SENS-S; REPRO (UNCERT); AQUATOX

**Summary of Assessment:**



**Fate:****Fate Summary:** T-11-0012

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log Koc = 3.05 (E)

log Fish BCF = 3.04 (E)

log Fish BAF = 2.954 (E)

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Biodeg - Closed Btl): 62%/28d; Analog [REDACTED]: OECD 301F(Mano Resp): 75%/28d,

60%/10d; OECD 305(BCF): LogBCF=3.2(dry weight), 4.5(lipid weight).

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\*CEB FATE: Migration to ground water = slow-moderate

**Health:**

**Health Summary:** Absorption is poor all routes based on physical/chemical properties and analogs. There is concern for eye and skin irritation, more severe with repeated exposure ([REDACTED]); dermal sensitization ([REDACTED] and a submitted study); reproductive toxicity ([REDACTED]); possible liver toxicity ([REDACTED]) and lung toxicity in the form of chemical pneumonia. Low moderate concern.

**Test Data:** [REDACTED]

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): 28-day dermal study in rabbits dosed with 2 mL/kg, progressive skin irritation  
 dermal sensitizer in humans  
 rat oral devel/repro screen LOEL = 100 mg/kg, mild liver changes at all doses  
 rat oral devel/repro screen NOEL = 150 mg/kg, lower fertility index with a longer mean mating time at 1000  
 mg/kg  
 : mild eye irritation in rabbits; mild skin irritation in rabbits

**Ecotox:**

Test Organism	Test Type	Test End Point	Predicted	Measured	Comments
fish	96-h	LC50	0.19		
daphnid	48-h	LC50	0.14		
green algal	96-h	EC50	0.17		
fish	—	chronic value	0.026		
daphnid	—	chronic value	0.031		
algal	—	chronic value	0.17		
Sewage Sludge	3-h	EC50	—		
Sewage Sludge	—	Chronic Value	—		

**Ecotox Values Comments:** Predictions are based on SARs for neutral organic chemicals; SAR chemical class = hydrocarbon;  
 MW 142 (low weight); log Kow = 5.11 (EPI, low weight); liquid with mp = -33 C (M); S = 1.1 mg/L (P, low weight); pH7;  
 effective concentrations based on 100% active ingredients and nominal concentrations; DW hardness < 150.0 mg/L as CaCO3; and  
 DW TOC <2.0 mg/L;

Factors	Values	Comments
Assessment Factor	10	
Concentration of Concern (ppb) Acute		
Concentration of Concern (ppb) Chronic	3	
SARs	neutral organic chemicals	
SAR Class	hydrocarbon	new chemicals category: neutral organics

TSCA New Chemical Category	
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**Ecotox Factors Comments:**

**SAT Chair:** Becky Jones

**Fate assessor:** **Ecotox assessor:** **Health assessor:**